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ENERGY OF THE MOST LOOSELY BOUND ELECTRON FOR IONS OF COPPER, SILVER, AND GOLD

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ENERGY OF THE MOST LOOSELY BOUND ELECTRON FOR IONS OF COPPER, SILVER, AND GOLD

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Leonard H. Harris

ENERGY OF THE MOST LOOSELY BOUND ELECTRON FOR IONS OF COPPER, SILVER, AND GOLD

by

Leonard H. Harris

Captain, United States Army

Submitted in partial fulfilment of
the requirements for the degree of

MASTER OF SCIENCE

IN

PHYSICS

United States Naval Postgraduate School
Monterey, California

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This work is accepted as fulfilling
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ABSTRACT

This paper presents a new numerical method for solving Schroedinger's equation in radial form in order to get a set of wave functions for use as starting values in the solution of the Fock equation. As a necessary adjunct to the solution, an improved numerical method is given for calculating potentials for use in the Schroedinger equation. Finally, a method is outlined for solving the Fock equation numerically, using the wave functions obtained above as starting values.

ENERGY OF THE MOST LOOSELY BOUND ELECTRON FOR IONS OF COPPER, SILVER, AND GOLD

If the energy and distance from the nucleus of the most loosely bound electron in an ion of a metallic lattice can be found, it is possible to use this data to calculate certain physical constants of the metal, e.g. the elastic constants.

Wigner and Seitz[1] have shown how to find this binding energy, neglecting exchange forces, by solving Schroedinger's equation in radial form:

$$(1) \qquad -\frac{\hbar^2}{2m}\frac{d^2R}{dr^2} + [V(r) - E]R = 0$$

for various values of E. It is found that for each such value of E there are several radii at which the condition

$$(2) \qquad \frac{dR}{dr} = \frac{R}{r}$$

is satisfied. Most of these points are very close to the nucleus and are essentially the same for all values of E. If the outer two radii are plotted against E a curve results which exhibits a minimum. It is this minimum which gives the required data.

Fuchs[2] has extended the procedure to take into account exchange forces. His method involves solving the Fock equation:[3]

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[1] E. Wigner and Seitz, F., Phys. Rev., 43, 804 (1933)

[2] K. Fuchs, Proc. Roy. Soc., A, 131, 585 (1935)

[3] E. Fock, Zeits. F. Physik, 81, 195 (1933)

$$(3)\quad -\frac{\hbar^2}{2m}\frac{d^2R}{dr^2}+[V(r)-E]R-\int_0^\infty G(r,r')R(r')dr'=0\ .$$

The most practical method for solving this equation is first to solve equation (1) and then use the wave functions obtained to evaluate the integral in (3). This makes the right side a function of the independent variable instead of zero. When this resulting equation is solved the new wave functions are then used to re-evaluate the integral and the procedure is repeated as required.

As the first approximation, then, a solution of (1) is needed. To get it, it is necessary first to calculate the values of V to be used.

From the work of Hartree and others[4], tables of values of Z, the effective charge, are available as functions of ρ, the radius measured from the surface of the nucleus. These values have been accepted in this paper, although there may be errors in them since most were calculated by hand before the era of the electronic computer. The required values of v, however, were recalculated, where

$$(4)\qquad v=\frac{Z_p}{\rho}$$

and Z_p is the effective nuclear charge for potential which is different from Z. The values of v were calculated by

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[4] D. Hartree, Proc. Roy. Soc., A, 141, 282 (1933)
A. Douglas, Hartree D., and Runciman, W. Proc. Cambridge Phil. Soc., 51, 486 (1955)
M. Black, Manchester Memoirs, 79, 29 (1934)

integrating the field intensity

$$(5)\qquad \left(\frac{Z_\rho}{\rho}\right)_{\rho=\rho_2} = v(\rho_2) = v(\rho_1) + \int_{\rho_1}^{\rho_2} \frac{Z(r)}{r^2}\,dr \,.$$

The usual method[5] of calculating v is to solve the differential equation

$$(6)\qquad \frac{dZ_\rho}{d\rho} = \frac{Z_\rho - Z}{\rho}$$

by Euler's method, which is simple but inaccurate. It can be shown[6] that the error is of the order of

$$(7)\qquad \epsilon = \frac{(\rho_1-\rho_2)^2}{2}\left(\frac{d^2 Z_\rho}{d\rho^2}\right)_{\rho=\rho_1} \,.$$

Some simple algebra and substitution reduces this expression to

$$(8)\qquad \epsilon = \frac{(\rho_1-\rho_2)}{2\rho_1}\left[Z(\rho_2) - Z(\rho_1)\right]$$

since Z is assumed to be linear between any two adjacent radii. Graph 1 gives the relative % error for Cu^+ resulting from this calculation. It is large enough so that a more sophisticated method of solution, equation (5), was decided upon. The evaluation was done using a Gaussian 3-point quadrature formula, which is based on the assumption that between any two neighboring radii Z is approximated by a third degree polynomial.

To evaluate the integral in (5),

$$(9)\qquad A(\rho_2) = \int_{\rho_1}^{\rho_2} \left[\frac{Z(r)}{r^2}\right] dr$$

[5] D. Hartree, Proc. Cambridge Phil. Soc., 24, 114 (1928)

[6] Kunz, K., Numerical Analysis, McGraw-Hill, N.Y., 1957, pgs 177-8

it is first necessary to normalize the limits to the range 0 to 1 in order to use readily available values of the Gaussian coefficients. This can be done by the substitution

$$(10)\qquad u = \frac{1}{2}\left(\frac{2r-(\rho_1+\rho_2)}{\rho_2-\rho_1}+1\right).$$

Equation (9) then becomes

$$(11)\qquad A(\rho_2) = 4(\rho_2-\rho_1)\int_0^1 \frac{z\left(\frac{(2u-1)(\rho_2-\rho_1)+(\rho_1+\rho_2)}{2}\right)}{(2u-1)(\rho_2-\rho_1)+(\rho_1+\rho_2)^2}\,du .$$

The coefficients for the Gauss 3-point formula are

$$(12)\qquad \left\{\begin{array}{ll} u_0 = .11270167 & W_0 = \frac{5}{18} \\ u_1 = .5 & W_1 = \frac{4}{9} \\ u_2 = .88729833 & W_2 = \frac{5}{18} \end{array}\right\}.$$

Thus, (11) becomes

$$(13)\quad A(\rho_2) = \frac{2(\rho_2-\rho_1)}{9}\left[5\left\{\frac{z\left(\frac{\alpha\rho_1+\beta\rho_2}{2}\right)}{(\alpha\rho_1+\beta\rho_2)^2}+\frac{z\left(\frac{\beta\rho_1+\alpha\rho_2}{2}\right)}{(\beta\rho_1+\alpha\rho_2)^2}\right\}+8\,\frac{z\left(\frac{\rho_1+\rho_2}{2}\right)}{(\rho_1+\rho_2)^2}\right.$$

where

$$(14)\qquad \alpha = 1.77459666\ ; \quad \beta = .22540334 .$$

It can be shown[7] that the error is of the order of

$$(15)\quad \epsilon = \frac{1}{7}\left\{\frac{\rho_2-\rho_1}{2}\left[f(\rho_1)+f(\rho_2)\right]-A(\rho_2)-\left(\frac{\rho_2-\rho_1}{2}\right)^2\sum_{i=0}^{2}W_i u_i f'(u_i)\right\}$$

where f represents the integrand in (9). The magnitude of the relative error for Cu^+ is plotted in Graph 1. It is never greater than .25%

To use (13) it is necessary to develop an interpolation

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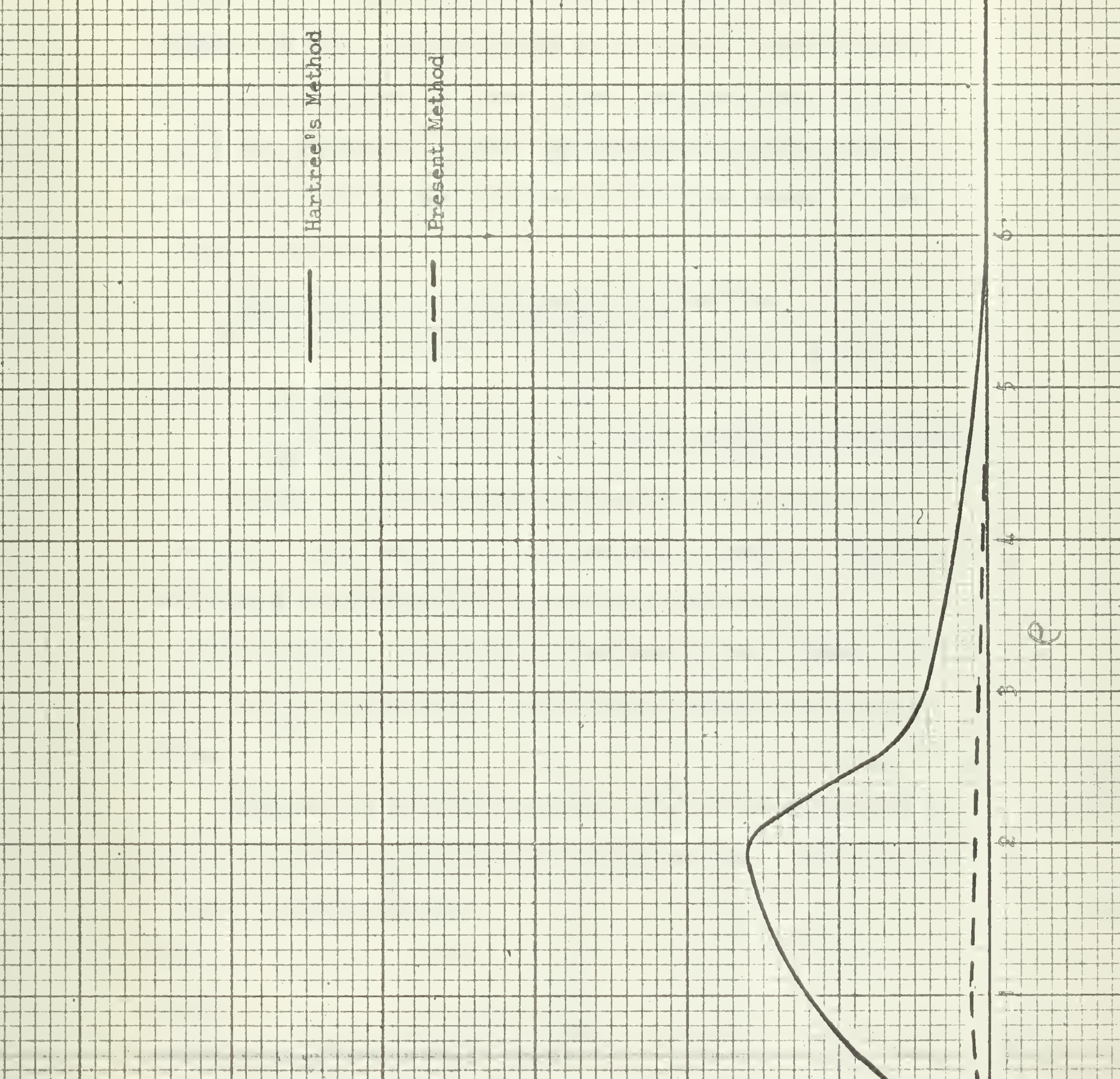
[7] Lanczos, C., Applied Analysis, Prentice Hall, N.J., 1956, pgs 404-7

GRAPH 1
% Relative Error Vs ρ



formula for calculating the 3 numerators on the right from the available table of values of Z. This has been done using a Gregory-Newton second degree divided difference interpolation formula. A third degree formula which would be consonant with the basic assumption involved in the Gaussian 3-point method would have increased the labor of programming significantly and would have made no difference in the final result, to the limits of accuracy retained.

The resulting three formulas are of the form

$$Z\left(\frac{\alpha\rho_1+\beta\rho_2}{2}\right)=Z(\rho_0)+\frac{\left[\frac{\alpha\rho_1+\beta\rho_2}{2}-\rho_0\right]}{(\rho_0-\rho_1)}\left[Z(\rho_0)-Z(\rho_1)\right]$$

(16)

$$+\frac{\left[\frac{\alpha\rho_1+\beta\rho_2}{2}-\rho_0\right]\left[\frac{\alpha\rho_1+\beta\rho_2}{2}-\rho_1\right]}{(\rho_0-\rho_1)(\rho_1-\rho_2)(\rho_0-\rho_2)}\left\{\left[Z(\rho_0)-Z(\rho_1)\right](\rho_1-\rho_2)-\left[Z(\rho_1)-Z(\rho_2)\right](\rho_0-\rho_1)\right\}.$$

Appendix 1 gives the CDC-1604 program for calculating v, starting at ρ_0 =6 Bohr radii and proceeding inward. v(ρ_1) is calculated by equation (42) for ρ_1 =5.5 Bohr radii as -.18181818181818. The first v calculated by the program is that for ρ_2 =5 Bohr radii. The values obtained are given in Table 1.

Equation (1) can now be solved. It is first desireable to write it in terms of Bohr radii and Rydberg energy units to get a dimensionless equation.

Let

(17) $$\rho=\frac{r}{a_o}$$

where a_o is a Bohr radius. Then

(18) $$\frac{d^2R}{dr^2}=\frac{1}{a_o^2}\frac{d^2R}{d\rho^2}$$

TABLE I

r	Cu^+		Ag^+		Au^+	
	Z	ν	Z	ν	Z	ν
.000	29.000		47.00		79.00	
.002			47.00	- 13910.		
.004			46.99	- 7438.		
.005	28.992	- 5668.2				
.006			46.95	- 4987.		
.008			46.91	- 3705.		
.010	28.948	- 2769.7	46.85	- 2919.		
.015	28.875	- 1805.0	46.63	- 1945.		
.020	28.759	- 1324.4	46.36	- 1438.	77.53	- 3502.
.025	28.615	- 1037.3	46.06	- 1129.		
.030	28.451	- 847.07	45.78	- 920.6		
.035	28.280	- 711.96	45.50	- 771.6		
.04	28.106	- 611.27	45.25	- 659.8	75.53	- 1573.
.05	27.765	- 471.60	44.73	- 509.6		
.06	27.451	- 379.58	44.20	- 409.2	72.86	- 953.3
.07	27.161	- 314.57	43.62	- 337.8		
.08	26.884	- 266.30	42.96	- 284.7	70.14	- 655.6
.09	26.608	- 229.14	42.26	- 243.8		
.10	26.320	- 199.71	41.52	- 211.6	67.76	- 483.1
.11			40.78	- 185.7		
.12	25.689	- 156.27	40.04	- 164.5	65.41	- 371.9
.14	24.977	- 126.05	38.71	- 132.8	62.92	- 295.3
.16	24.209	- 104.07	37.53	- 109.5	60.31	- 240.3
.18	23.413	- 87.533	36.48	- 91.81	57.75	- 199.4

TABLE I (Continued)

	Cu^+		Ag^+		Au^+	
r	Z	v	Z	v	Z	v
.20	22.646	- 74.745	35.48	- 77.99	55.44	- 168.0
.22	21.929	- 64.625	34.48	- 66.97	53.40	- 143.3
.24	21.279	- 56.452	33.43	- 58.07	51.66	- 123.4
.26	20.699	- 49.733	32.31	- 50.78	50.09	- 107.1
.28	20.187	- 44.124	31.16	- 44.76	48.62	- 93.55
.30	19.736	- 39.379	29.98	- 39.75	47.13	- 82.14
.32			28.80	- 35.53	45.62	- 72.47
.34			27.66	- 31.95	44.05	- 64.21
.35	18.791	- 30.224				
.36			26.57	- 28.89	42.36	- 57.15
.38			25.55	- 26.24	40.65	- 51.08
.40	17.964	- 23.650	24.61	- 23.96	38.94	- 45.84
.45	17.114	- 18.763	22.65	- 19.48	34.73	- 35.65
.50	16.193	- 15.050	21.16	- 16.06	30.96	- 28.41
.55	15.196	- 12.189	20.04	- 13.37	27.82	- 23.12
.60	14.153	- 9.963	19.13	- 11.23	25.33	- 19.12
.65					23.34	- 16.03
.7	12.051	- 6.851	17.58	- 8.124	21.73	- 13.57
.8	10.119	- 4.890	15.94	- 5.994	19.23	- 9.938
.9	8.467	- 3.616	14.21	- 4.505	17.13	- 7.419
1.0	7.110	- 2.763	12.50	- 3.451	15.19	- 5.625
1.1	6.018	- 2.175	10.87	- 2.695	13.34	- 4.334
1.2	5.148	- 1.758	9.40	- 2.15	11.68	- 3.391
1.3	4.455	- 1.454			10.18	- 2.695

TABLE I (Continued)

	Cu^+		Ag^+		Au^+	
r	Z	υ	Z	υ	Z	υ
1.4	3.896	- 1.228	7.03	- 1.47	8.88	- 2.14
1.5					7.76	- 1.78
1.6	3.070	- .9275	5.31	- 1.08	6.78	- 1.48
1.8	2.507	- .7387	4.11	- .833	5.25	- 1.08
2.0	2.107	- .6132	3.26	- .674	4.14	- .825
2.2	1.817	- .5256	2.65	- .566	3.34	- .658
2.4	1.606	- .4617	2.21	- .490	2.72	- .547
2.6	1.448	- .4133	1.89	- .434	2.28	- .468
2.8	1.330	- .3755	1.65	- .391	1.95	- .411
3.0	1.243	- .3451	1.48	- .358	1.70	- .368
3.2	1.179	- .3201	1.35	- .331	1.52	- .335
3.4	1.130	- .2990	1.25	- .305	1.38	- .309
3.6	1.095	- .2808	1.19	- .285	1.28	- .287
3.8	1.068	- .2651	1.13	- .267	1.21	- .269
4.0	1.050	- .2512	1.10	- .252	1.15	- .253
4.5	1.022	- .2226	1.04	- .223	1.07	- .223
5.0	1.008	- .2001	1.02	- .200	1.03	- .200
5.5	1.003	- .1818	1.01	- .182	1.01	- .182
6.0	1.001	- .1667	1.00	- .167	1.00	- .167

so that (1) becomes

(19) $$\frac{d^2R}{d\rho^2} + \frac{2ma_0^2}{\hbar^2}(E - V)R = 0 .$$

If E is in Rydberg units we can write

(20) $$E = \frac{me^4}{2\hbar^2}\epsilon ,$$

where ϵ is a dimensionless number, since a Rydberg unit is given by

(21) $$Rch = \frac{me^4}{2\hbar^2} .$$

Also, if

(22) $$v = \frac{Z_p}{\rho}$$

then

$$V = (v)\left(\frac{e^2}{a_0}\right)$$

(23)

Inserting (20) and (23) in (19),

(24) $$\frac{d^2R}{d\rho^2} + \frac{2ma_0^2}{\hbar^2}\left[\frac{me^4}{2\hbar^2}\epsilon - (v)\left(\frac{e^2}{a_0}\right)\right]R = 0 .$$

But,

(25) $$a_0 = \frac{\hbar^2}{me^2}$$

so (24) becomes

(26) $$\frac{d^2R}{d\rho^2} + \left[\epsilon - \mathcal{Q}(\rho)\right]R = 0$$

where

(27) $$\mathcal{Q} = 2v \quad .$$

Equation (26) can be solved readily using a Runge-Kutta 4th order approximation. Let

(28) $$y = \frac{dR}{d\rho} \quad .$$

Then

(29) $$\frac{dy}{d\rho} = \frac{d^2R}{d\rho^2}$$

and the set of equations to be solved is

(30) $$\left\{ \begin{aligned} \frac{dy}{d\rho} &= [\mathcal{Q}(\rho) - \epsilon] R \\ \frac{dR}{d\rho} &= y \end{aligned} \right\} \quad .$$

The formulas for the solution are

(31) $$\left\{ \begin{aligned} \Delta R &= \frac{1}{6}\left(\Delta' R + 2\Delta'' R + 2\Delta''' R + \Delta^{IV} R\right) \\ \Delta y &= \frac{1}{6}\left(\Delta' y + 2\Delta'' y + 2\Delta''' y + \Delta^{IV} y\right) \end{aligned} \right\}$$

where the quantities on the right are calculated in the following order:

(32) $$\left\{ \begin{aligned} \Delta' R &= f(\rho_0, R_0, y_0)h \\ \Delta' y &= g(\rho_0, R_0, y_0)h \\ \Delta'' R &= f(\rho_0 + \tfrac{1}{2}h, R_0 + \tfrac{1}{2}\Delta' R, y_0 + \tfrac{1}{2}\Delta' y)h \\ \Delta'' y &= g(\rho_0 + \tfrac{1}{2}h, R_0 + \tfrac{1}{2}\Delta' R, y_0 + \tfrac{1}{2}\Delta' y)h \\ \Delta''' R &= f(\rho_0 + \tfrac{1}{2}h, R_0 + \tfrac{1}{2}\Delta'' R, y_0 + \tfrac{1}{2}\Delta'' y)h \\ \Delta''' y &= g(\rho_0 + \tfrac{1}{2}h, R_0 + \tfrac{1}{2}\Delta'' R, y_0 + \tfrac{1}{2}\Delta'' y)h \\ \Delta^{IV} R &= f(\rho_0 + h, R_0 + \Delta''' R, y_0 + \Delta''' y)h \\ \Delta^{IV} y &= g(\rho_0 + h, R_0 + \Delta''' R, y_0 + \Delta''' y)h \end{aligned} \right\} \quad .$$

Here,

(33) $$\left\{ \begin{aligned} f &= y \\ g &= [\mathcal{Q}(\rho) - \epsilon] R \\ h &= \rho_1 - \rho_0 \end{aligned} \right\} \quad .$$

After making the calculations (32) and inserting in formulas (31) we get

$$\Delta R = \frac{h}{6}\Big\{6y_0 + \mathcal{Q}(\rho_0)R_0h - 3\epsilon R_0h + 2\mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}\right)R_0h + \mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}\right)y_0h^2 - \epsilon y_0h^2 + \frac{R_0h^3}{4}\left[\mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}\right)-\epsilon\right]\left[\mathcal{Q}(\rho_0)-\epsilon\right]\Big\}$$

(34) $$\Delta y = \frac{h}{6}\Big\{\mathcal{Q}(\rho_0)R_0 - 6\epsilon R_0 + 4\mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}\right)R_0 + 2\mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}\right)y_0h - 3\epsilon y_0h + \frac{R_0h^2}{2}\left[\mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}\right)-\epsilon\right]\left[\mathcal{Q}(\rho_0)-\epsilon\right] + \mathcal{Q}(\rho_1)R_0 + \mathcal{Q}(\rho_1)y_0h + \frac{h^2}{2}\left[\mathcal{Q}(\rho_1)-\epsilon\right]\left[\mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}-\epsilon\right]\left[R_0+\tfrac{1}{2}y_0h\right]\Big\} .$$

As before, $\mathcal{Q}\left(\frac{\rho_0+\rho_1}{2}\right)$ is calculated using a Gregory-Newton second degree divided difference interpolation formula of the same form as equation (16).

Since equations (34) give only successive increments in R and y it is necessary to obtain starting values for each.

Assume that near the origin

(35) $$R = b_0 + b_1\rho + b_2\rho^2 + \ldots .$$

Also, for small ρ ,

(36) $$\mathcal{Q} = -\frac{2\bar{Z}}{\rho}$$

where $\bar{Z}$ is the complete charge on the ion. Differentiating (35) twice and inserting it and (36) in (26) gives

(37) $$(2b_2 + \epsilon b_0 + 2\bar{Z}b_1) + (6b_3 + \epsilon b_1 + 2\bar{Z}b_2)\rho + (12b_4 + \epsilon b_2 + 2\bar{Z}b_3)\rho^2 + (20b_5 + \epsilon b_3 + 2\bar{Z}b_4)\rho^3 + \cdots + \frac{2\bar{Z}b_0}{\rho} = 0 .$$

Thus,

(38) $$\left\{\begin{array}{l} b_0 = 0 \\ b_2 = -\bar{Z}b_1 \\ b_3 = \frac{1}{6}(2\bar{Z}^2 - \epsilon)b_1 \\ \text{etc.} \end{array}\right\} .$$

For small , we want

(39) $$R(\delta\rho) \approx \delta\rho$$

Inserting (39) in (35)

(40) $$R(\delta\rho) = b_1(\delta\rho) + b_2(\delta\rho)^2 + \dots \approx b_1(\delta\rho)$$

so that $b_1 = 1$.

As starting values, let us calculate initial values for R and y at $\rho = .002$. Inserting the coefficients in (35)

(41) $$\left\{\begin{array}{l} R \approx \rho - Z\rho^2 + \frac{1}{6}(2Z^2 - \epsilon)\rho^3 \\ y \approx 1 - 2Z\rho + \frac{1}{2}(2Z^2 - \epsilon)\rho^2 \end{array}\right\} .$$

We can ignore ϵ compared with $2Z^2$. Then the starting values for any ϵ are

	Cu^+	Ag^+	Au^+
R	.002	.002	.002
y	.887	.821	.709

The CDC-1604 program for the calculation is in Appendix 2. The magnitude of the initial energy was set at .4 in each case and increased in increments of .01 to 1.0 (to 1.6 for gold). The potentials for $\rho = .002$ were calculated from equation (36). Potentials for $\rho > 6$ were calculated from

(42) $$v = \frac{1}{\rho} .$$

The wave functions from this calculation are intended merely for starting values in equation (3), so no great accuracy is required. The error[8] is of the order of h^5. Only a sample

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[8] Kunz, K., op. cit., pg 188

curve of R vs ρ is shown for each metal, that for the energy value at which the minimum of the curve of ϵ vs ρ was achieved. This is given in Graph 2. The curves of ϵ vs ρ are shown in Graph 3.

To solve (3) it may first be put in dimensionless form:

$$\frac{d^2R}{d\rho^2} + \left[\epsilon - \partial(\rho)\right]R + 2\int_0^\infty G(\rho,r)R(r)\,dr = 0 \tag{43}$$

where

$$G(\rho,r) = \sum_m \sum_l K_l f_{m,l}(\rho) f_{m,l}(r) \tag{44}$$

and

$$K_l = \left\{ \begin{array}{ll} \dfrac{r^{l-1}}{\rho^l} & r < \rho \\ \dfrac{\rho^{l-1}}{r^l} & r > \rho \end{array} \right\} \tag{45}$$

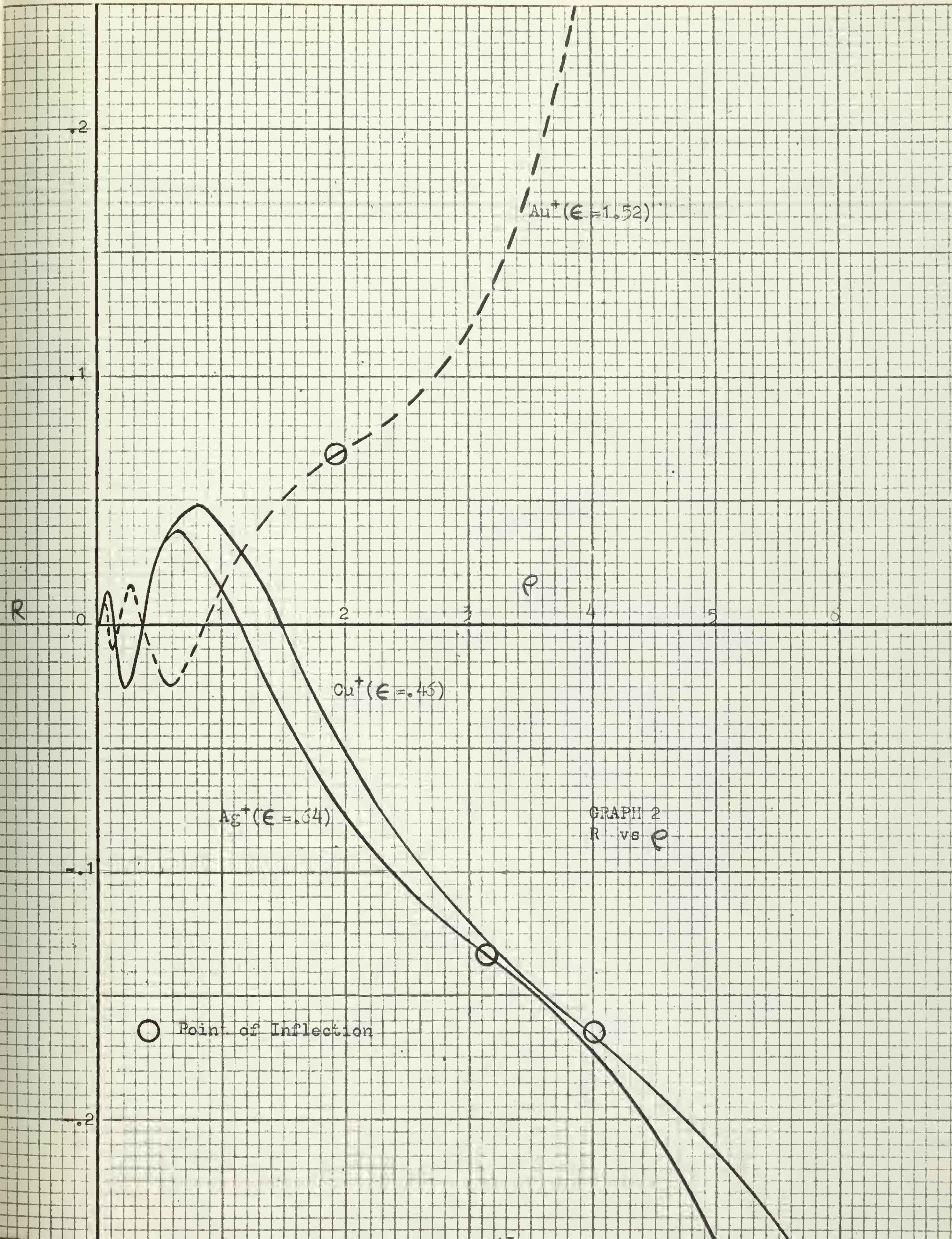
Here the $f_{n,1}$ refer to the wave functions for the individual electronic shells. These are available (cf note 4).

For Cu⁺, the filled shells are the 1s, 2s, 2p, 3s, 3p, and 3d, corresponding to n,1 values of 10, 20, 21, 30, 31, 32. The integral then becomes (using $r < \rho$ as an example)

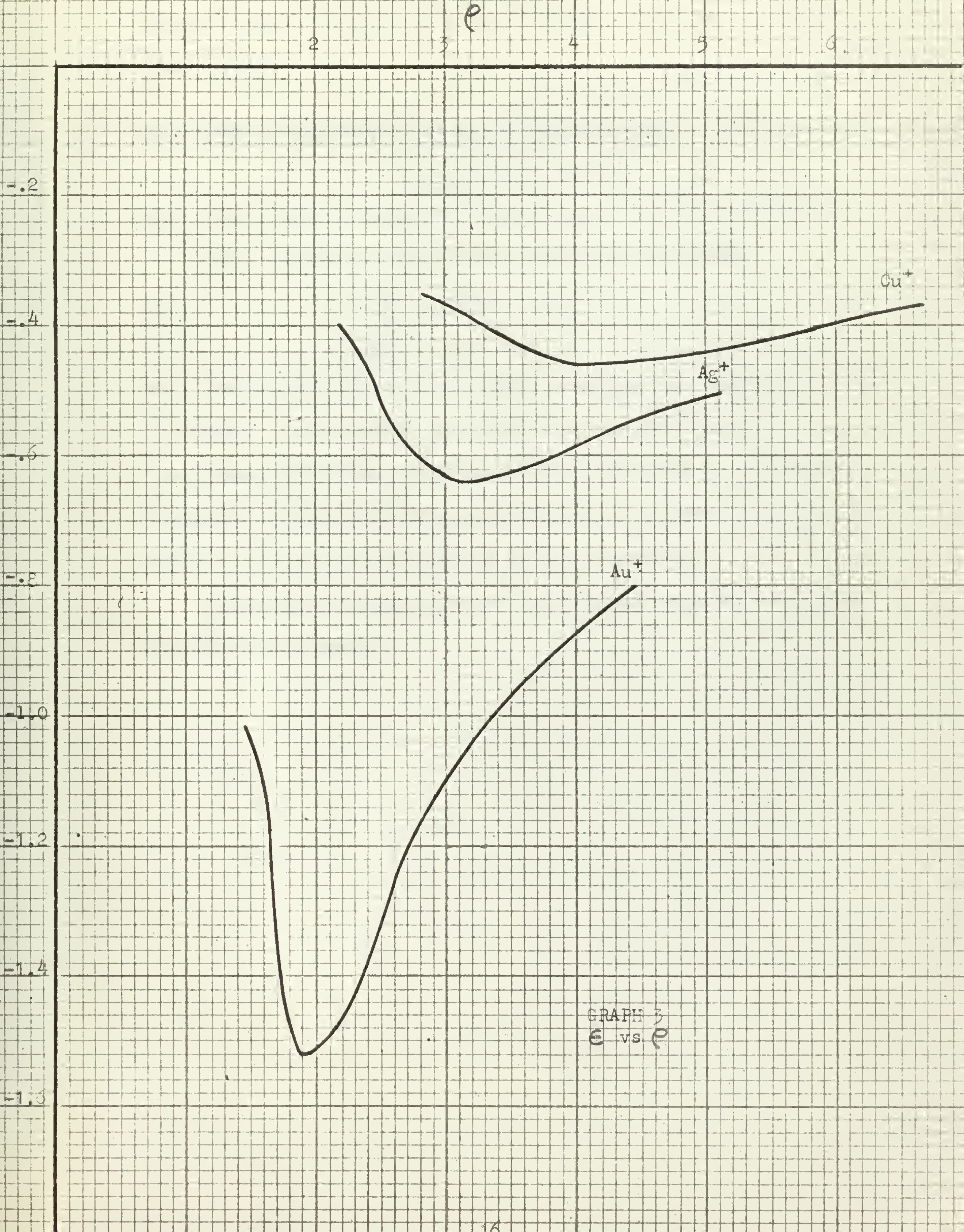
$$\begin{aligned} \int_0^\infty G(\rho,r)R(r)\,dr &= f_{1,0}(\rho)\int_0^\infty \frac{f_{1,0}(r)}{r}R(r)\,dr + f_{2,0}(\rho)\int_0^\infty \frac{f_{2,0}(r)}{r}R(r)\,dr \\ &+ f_{3,0}(\rho)\int_0^\infty \frac{f_{3,0}(r)}{r}R(r)\,dr + \frac{f_{2,1}(\rho)}{\rho}\int_0^\infty f_{2,1}(r)R(r)\,dr \\ &+ \frac{f_{3,1}(\rho)}{\rho}\int_0^\infty f_{3,1}(r)R(r)\,dr + \frac{f_{3,1}(\rho)}{\rho^2}\int_0^\infty r f_{3,1}(r)R(r)\,dr \end{aligned} \tag{46}$$

and similarly for $r > \rho$.

All the integrals on the right can be evaluated using numerical methods with the wave functions calculated above as starting values, although the programming will be tedious.



GRAPH 2
R vs ρ



GRAPH 3
ε vs ρ

The integration, for all practical purposes, probably need not proceed beyond the range 0 to 6. The right hand side of (46) then becomes

$$(47)\quad F(\rho) = a_1 f_{1,0}(\rho) + a_2 f_{2,0}(\rho) + a_3 f_{3,0}(\rho) + a_4 f_{2,1}(\rho) + a_5 f_{3,1}(\rho) + a_6 f_{3,1}(\rho)$$

where the a's are the constants resulting from the integrations.

It is then necessary to solve the set of equations

$$(48)\quad \left\{ \begin{aligned} \frac{dy}{d\rho} &= [Q(\rho) - \epsilon] R + F(\rho) \\ \frac{dR}{d\rho} &= y \end{aligned} \right\}$$

by a Runge-Kutta approximation using equations (31) and (32) as before. The resulting wave functions are then used to re-evaluate the integrals on the right of (46) and so on. The procedure is terminated when succeeding sets of wave functions differ by less than the required degree of accuracy.

Unfortunately, there was not enough time available to write the CDC-1604 program.

CONCLUSIONS

The results obtained differ significantly from thoseof other investigators. For example, Fuchs calculated the minimum energy for copper as approximately .8, occurring at about 2.9 Bohr radii. He gives no estimate of his possible error, however.

Since the error in finding each increment in the method used here is of the order of h^5, the cumulative error in R to the radius at which the minimum occurs is in no case greater than .003. The accuracy of the method cannot be called into question, therefore.

There is always the possibility of a mistake in algebra or programming, such as the omission of a factor of two. Every step in the calculation has been checked over four times, and if there is such an error it must be very subtle in nature.

It should not be thought, however, that the results of previous investigators in this field are necessarily correct. They were calculating by hand, and the methods which they were forced to use were so oversimplified that reasonable accuracy was often impossible. Indeed, if the previous investigators (who all seem to have used the same methods) had been in error only .01 units for each increment of R, their total error could be very large.

APPENDICES

Note: Figures in the 2^d column refer to Ag^+ and in the 3^d column to Au^+, where different from the 1^{st} column, which is for Cu^+

APPENDIX I

```
        ORG    10000
STOR    EQU    11000
ANS     EQU    12000
VR1     EQU    11100
        LDA  0 VIN
        STA  0 VR1
SFT     ENI  1 00000
        ENI  2 00000
BEGIN   LDA  0 ALPHA
        FMU  1 RAD+1
        STA  0 STOR
        LDA  0 BETA
        FMU  1 RAD+2
        FAD  0 STOR
        STA  0 STOR
        FDV  0 TWO
        STA  0 STOR+1
        LDA  0 STOR
        FMU  0 STOR
        STA  0 STOR
        LDA  0 BETA
        FMU  1 RAD+1
        STA  0 STOR+2
        LDA  0 ALPHA
        FMU  1 RAD+2
```

```
FAD     0  STOR+2
STA     0  STOR+2
FDV     0  TWO
STA     0  STOR+3
LDA     0  STOR+2
FMU     0  STOR+2
STA     0  STOR+2
LDA     1  RAD+1
FAD     1  RAD+2
STA     0  STOR+4
FDV     0  TWO
STA     0  STOR+5
LDA     0  STOR+4
FMU     0  STOR+4
STA     0  STOR+4
LDA     1  ZETA
FSB     1  ZETA+1
STA     0  STOR+6
LDA     1  ZETA+1
FSB     1  ZETA+2
STA     0  STOR+7
LDA     1  RAD
FSB     1  RAD+1
STA     0  STOR+8D
LDA     1  RAD+1
FSB     1  RAD+2
STA     0  STOR+9D
```

```
LDA  1 RAD
FSB  1 RAD+2
STA  0 STOR+10D
LDA  0 STOR+6
FMU  0 STOR+9D
STA  0 STOR+11D
LDA  0 STOR+7
FMU  0 STOR+8D
STA  0 STOR+12D
LDA  0 STOR+11D
FSB  0 STOR+12D
STA  0 STOR+11D
LDA  0 STOR+8D
FMU  0 STOR+9D
FMU  0 STOR+10D
STA  0 STOR+9D
LDA  0 STOR+1
FSB  1 RAD
STA  0 STOR+13D
FDV  0 STOR+8D
FMU  0 STOR+6
STA  0 STOR+14D
LDA  0 STOR+1
FSB  1 RAD+1
FMU  0 STOR+13D
FDV  0 STOR+10D
FMU  0 STOR+11D
FAD  0 STOR+14D
FAD  1 ZETA
FDV  0 STOR
STA  0 STOR+1
```

```
LDA   0 STOR+3
FSB   1 RAD
STA   0 STOR+15D
FDV   0 STOR+8D
FMU   0 STOR+6
STA   0 STOR+16D
LDA   0 STOR+3
FSB   1 RAD+1
FMU   0 STOR+15D
FDV   0 STOR+10D
FMU   0 STOR+11D
FAD   0 STOR+16D
FAD   1 ZETA
FDV   0 STOR+2
FAD   0 STOR+1
FMU   0 FIVE
STA   0 STOR+3
STA   0 STOR+3
LDA   0 STOR+5
FSB   1 RAD
STA   0 STOR+17D
FDV   0 STOR+8D
FMU   0 STOR+6
STA   0 STOR+18D
LDA   0 STOR+5
FSB   0 RAD+1
```

```
        FMU  0 STOR+17D
        FDV  0 STOR+10D
        FMU  0 STOR+11D
        FAD  0 STOR+18D
        FAD  1 ZETA
        FDV  0 STOR+4
        FMU  0 FIGHT
        FAD  0 STOR+3
        FMU  0 TWO
        FDV  0 NINE
        STA  0 STOR+3
        LDA  1 RAD+2
        FSB  1 RAD+1
        FMU  0 STOR+3
        FAD  0 VR1
        STA  0 VR1
        LDQ  1 RAD+2
        STQ  2 ANS
        STA  2 ANS+1
        INI  2 00002
        ENI  0 00000
        ISK  1 53D          ISK  1  59D          ISK  1  49D
        SLJ  0 BEGIN
        ENI  3 00000
        ENI  4 ANS
CONV    SLJ  4 71000
```

```
      ENI  0 00000
      001  0 ANS
      006  0 0
      INI  4 00006
      ENA  4 00000
      SAU  0 CONV+1
      ENI  0 00000
      ISK  3 17D             ISK  3  19D             ISK  3  16D
      SLJ  0 CONV
      ENI  0 00000
      SLS  0 00000
VIN   DEC    -.18181818181818
ALPHA DEC    1.774596666
BETA  DEC    .22540334
TWO   DEC    2.
FIVE  DEC    5.
EIGHT DEC    8.
NINE  DEC    9.
RAD   DEC    6.
      DEC    5.5
      DEC    5.
      DEC    4.5
      DEC    4.
      DEC    3.8
      DEC    3.6
      DEC    3.4
```

```
DEC   3.2
DEC   3.
DEC   2.8
DEC   2.6
DEC   2.4
DEC   2.2
DEC   2.
DEC   1.8
DEC   1.6
DEC   1.4         DEC   1.4         DEC   1.5
DEC   1.3         DEC   1.2         DEC   1.4
DEC   1.2         DEC   1.1         DEC   1.3
DEC   1.1         DEC   1.0         DEC   1.2
DEC   1.          DEC    .9         DEC   1.1
DEC    .9         DEC    .8         DEC   1.
DEC    .8         DEC    .7         DEC    .9
DEC    .7         DEC    .6         DEC    .8
DEC    .6         DEC    .55        DEC    .7
DEC    .55        DEC    .5         DEC    .65
DEC    .5         DEC    .45        DEC    .6
DEC    .45        DEC    .4         DEC    .55
DEC    .4         DEC    .38        DEC    .5
DEC    .35        DEC    .36        DEC    .45
DEC    .3         DEC    .34        DEC    .4
DEC    .28        DEC    .32        DEC    .38
DEC    .26        DEC    .3         DEC    .36
```

```
      DEC  .24
      DEC  .22
      DEC  .2
      DEC  .18
      DEC  .16
      DEC  .14
      DEC  .12
      DEC  .1
      DEC  .09
      DEC  .08
      DEC  .07
      DEC  .06
      DEC  .05
      DEC  .04
      DEC  .035
      DEC  .03
      DEC  .025
      DEC  .02
      DEC  .015
      DEC  .01
      DEC  .005
      DEC  0
ZETA  DEC  1.001
      DEC  1.003
      DEC  1.008
      DEC  1.022
      DEC  .28
      DEC  .26
      DEC  .24
      DEC  .22
      DEC  .2
      DEC  .18
      DEC  .16
      DEC  .14
      DEC  .12
      DEC  .11
      DEC  .1
      DEC  .09
      DEC  .08
      DEC  .07
      DEC  .06
      DEC  .05
      DEC  .04
      DEC  .035
      DEC  .03
      DEC  .025
      DEC  .02
      DEC  .015
      DEC  .01
      DEC  .008
      DEC  .006
      DEC  .004
      DEC  .34
      DEC  .32
      DEC  .3
      DEC  .28
      DEC  .26
      DEC  .24
      DEC  .22
      DEC  .2
      DEC  .18
      DEC  .16
      DEC  .14
      DEC  .12
      DEC  .1
      DEC  .08
      DEC  .06
      DEC  .04
      DEC  .02
      DEC  0
ZETA  DEC  1.
      DEC  1.01
      DEC  1.03
      DEC  1.07
      DEC  1.15
      DEC  1.21
      DEC  1.28
      DEC  1.38
```

```
      DEC    1.050
      DEC    1.068
      DEC    1.095
      DEC    1.130
      DEC    1.179
      DEC    1.243
      DEC    1.330
      DEC    1.448
      DEC    1.606
      DEC    1.817
      DEC    2.107
      DEC    2.507
      DEC    3.070
      DEC    3.896
      DEC    4.455
      DEC    5.148
      DEC    6.018
      DEC    7.110
      DEC    8.467
      DEC   10.119
      DEC   12.051
      DEC   14.153
      DEC   15.196
      DEC   16.193
      DEC   17.114
      DEC   17.964
```

```
      DEC    .002
      DEC    0
ZETA  DEC    1
      DEC    1.01
      DEC    1.02
      DEC    1.04
      DEC    1.10
      DEC    1.13
      DEC    1.19
      DEC    1.25
      DEC    1.35
      DEC    1.48
      DEC    1.65
      DEC    1.89
      DEC    2.21
      DEC    2.65
      DEC    3.26
      DEC    4.11
      DEC    5.31
      DEC    7.03
      DEC    9.40
      DEC   10.87
      DEC   12.5
      DEC   14.21
      DEC   15.94
      DEC   17.58
```

```
      DEC    1.52
      DEC    1.70
      DEC    1.95
      DEC    2.28
      DEC    2.72
      DEC    3.34
      DEC    4.14
      DEC    5.25
      DEC    6.78
      DEC    7.76
      DEC    8.88
      DEC   10.18
      DEC   11.68
      DEC   13.34
      DEC   15.19
      DEC   17.13
      DEC   19.23
      DEC   21.73
      DEC   23.34
      DEC   25.33
      DEC   27.82
      DEC   30.96
      DEC   34.73
      DEC   38.94
      DEC   40.65
      DEC   42.36
```

```
DEC  18.791

DEC  19.736

DEC  20.187

DEC  20.699

DEC  21.279

DEC  21.929

DEC  22.646

DEC  23.413

DEC  24.209

DEC  24.977

DEC  25.689

DEC  26.320

DEC  26.608

DEC  26.884

DEC  27.161

DEC  27.451

DEC  27.765

DEC  28.106

DEC  28.280

DEC  28.451

DEC  28.615

DEC  28.759

DEC  28.875

DEC  28.948

DEC  28.992

DEC  29.000
END
```

```
DEC  19.13

DEC  20.04

DEC  21.16

DEC  22.65

DEC  24.61

DEC  25.55

DEC  26.57

DEC  27.66

DEC  28.8

DEC  29.98

DEC  31.16

DEC  32.31

DEC  33.43

DEC  34.48

DEC  35.48

DEC  36.48

DEC  37.53

DEC  38.71

DEC  40.04

DEC  40.78

DEC  41.52

DEC  42.26

DEC  42.96

DEC  43.62

DEC  44.20

DEC  44.73
DEC  45.25
```

```
DEC  44.05

DEC  45.62

DEC  47.13

DEC  48.62

DEC  50.09

DEC  51.66

DEC  53.40

DEC  55.44

DEC  57.75

DEC  60.31

DEC  62.92

DEC  65.41

DEC  67.76

DEC  70.14

DEC  72.86

DEC  75.53

DEC  77.53

DEC  79.

END
```

```
DEC  45.5
DEC  45.78
DEC  46.06
DEC  46.36
DEC  46.63
DEC  46.85
DEC  46.91
DEC  46.95
DEC  46.99
DEC  47.
DEC  47.
END
```

Note 1: Library subroutine DECOF 1 must be placed in memory starting at cell 71000. Output will be on magnetic tape unit 4.

Note 2: Program prints ρ and ν. Two to a line in decimal floating point.

APPENDIX II

```
        REM   SCHR EQ BY RK METHOD
        ORG   20000
VALUE   EQU   22000
STOR    EQU   21000
WYE     EQU   21600
ARE     EQU   21650
ENERGY  EQU   21700
        LDA 0 INEN
        STA 0 ENERGY
        ENI 3 00000
        ENI 0 00000
BEGIN   ENI 1 00000
        ENI 2 00000
        LDA 0 RIN
        STA 0 ARE
        LDA 0 YIN
        STA 0 WYE
RETURN  LDA 1 RAD
        FSB 1 RAD+1
        STA 0 STOR
        LDA 1 RAD
        FSB 1 RAD+2
        STA 0 STOR+1
        LDA 1 RAD+1
        FAD 1 RAD+2
```

```
FSB   1 RAD
FSB   1 RAD
STA   0 STOR+2
LDA   1 POT+1
FSB   1 POT+2
FMU   0 STOR+2
FDV   0 FOUR
FDV   0 STOR+1
STA   0 STOR+3
LDA   1 POT
FSB   1 POT+1
FMU   0 STOR+2
FMU   0 STOR+2
FDV   0 FOUR
FDV   0 STOR
FDV   0 STOR+1
STA   0 STOR+4
LDA   1 POT
FSB   0 STOR+4
FAD   0 STOR+3
STA   0 STOR+5
LDA   1 RAD+1
FSB   1 RAD
STA   0 STOR+6
FMU   0 STOR+6
STA   0 STOR+7
```

```
FMU   0 STOR+6
STA   0 STOR+8D
LDA   1 POT
FSB   0 ENERGY
STA   0 STOR+9D
LDA   0 STOR+5
FSB   0 ENERGY
FMU   0 STOR+9D
FMU   0 STOR+8D
FMU   0 ARE
FDV   0 FOUR
STA   0 STOR+10D
LDA   0 ENERGY
FMU   0 WYE
FMU   0 STOR+7
STA   0 STOR+11D
LDA   0 STOR+5
FMU   0 WYE
FMU   0 STOR+7
STA   0 STOR+12D
LDA   0 STOR+5
FMU   0 ARE
FMU   0 STOR+6
FMU   0 TWO
STA   0 STOR+13D
LDA   0 ENERGY
```

```
FMU   0 THREE
FMU   0 ARE
FMU   0 STOR+6
STA   0 STOR+14D
LDA   1 POT
FMU   0 ARE
FMU   0 STOR+6
STA   0 STOR+15D
LDA   0 WYE
FMU   0 SIX
FAD   0 STOR+15D
FSB   0 STOR+14D
FAD   0 STOR+13D
FAD   0 STOR+12D
FSB   0 STOR+11D
FAD   0 STOR+10D
FMU   0 STOR+6
FDV   0 SIX
STA   0 STOR+16D
LDA   1 POT+1
FMU   0 WYE
FMU   0 STOR+6
STA   0 STOR+18D
LDA   0 WYE
FMU   0 STOR+6
FDV   0 TWO
```

```
FAD   0 ARE
STA   0 STOR+19D
LDA   0 STOR+5
FSB   0 ENERGY
STA   0 STOR+20D
LDA   1 POT+1
FSB   0 ENERGY
FMU   0 STOR+20D
FMU   0 STOR+19D
FMU   0 STOR+7
FDV   0 TWO
STA   0 STOR+21D
LDA   0 ENERGY
FMU   0 ARE
FMU   0 SIX
STA   0 STOR+22D
LDA   1 POT+1
FMU   0 ARE
STA   0 STOR+23D
LDA   1 POT
FSB   0 ENERGY
STA   0 STOR+24D
LDA   0 STOR+5
FSB   0 ENERGY
FMU   0 STOR+24D
FMU   0 ARE
```

```
FMU  0 STOR+7
FDV  0 TWO
STA  0 STOR+25D
LDA  0 ENERGY
FMU  0 WYE
FMU  0 STOR+6
FMU  0 THREE
STA  0 STOR+26D
LDA  0 STOR+5
FMU  0 WYE
FMU  0 STOR+6
FMU  0 TWO
STA  0 STOR+27D
LDA  0 STOR+5
FMU  0 ARE
FMU  0 FOUR
STA  0 STOR+28D
LDA  1 POT
FMU  0 ARE
FSB  0 STOR+22D
FAD  0 STOR+28D
FAD  0 STOR+27D
FSB  0 STOR+26D
FAD  0 STOR+25D
FAD  0 STOR+23D
FAD  0 STOR+21D
FAD  0 STOR+18D
```

```
         FMU  0 STOR+6
         FDV  0 SIX
         FAD  0 WYE
         STA  0 WYE
         STA  2 VALUE+3
         LDA  1 RAD+1
         STA  2 VALUE
         LDA  0 STOR+16D
         FAD  0 ARE
         STA  0 ARE
         STA  2 VALUE+1
         FDV  1 RAD+1
         STA  2 VALUE+2
         INI  2 00004
         ENI  0 00000
         ISK  1 56D          ISK  1 59D          ISK  1 52D
         SLJ  0 RETURN
         ENI  4 00000
         ENI  5 VALUE
CONV     SLJ  4 71000
         ENI  0 00000
         001  0 VALUE
         004  0 0
         INI  5 00004
         ENA  5 00000
         SAU  0 CONV+1
```

```
       ENI  0 00000
       ISK  4 56D              ISK  4 59D              ISK  4 52D
       SLJ  0 CONV
       LDA  0 ENERGY
       FAD  0 DELEN
       STA  0 ENERGY
       ENI  0 00000
       ISK  3 00075                                    ISK  3 00170
       SLJ  0 BEGIN
       ENI  0 00000
       SLS  0 00000
INEN   DEC  -.4
TWO    DEC  2.
THREE  DEC  3.
FOUR   DEC  4.
SIX    DEC  6.
DELEN  DEC  -.01
RIN    DEC  .002
YIN    DEC  .887               DEC  .821               DEC  .709
RAD    DEC  .002
       DEC  .005               DEC  .004               DEC  .02
       DEC  .01                DEC  .006               DEC  .04
       DEC  .015               DEC  .008               DEC  .06
       DEC  .02                DEC  .01                DEC  .08
       DEC  .025               DEC  .015               DEC  .1
       DEC  .03                DEC  .02                DEC  .12
```

```
DEC     .035
DEC     .04
DEC     .05
DEC     .06
DEC     .07
DEC     .08
DEC     .09
DEC     .1
DEC     .12
DEC     .14
DEC     .16
DEC     .18
DEC     .2
DEC     .22
DEC     .24
DEC     .26
DEC     .28
DEC     .3
DEC     .35
DEC     .4
DEC     .45
DEC     .5
DEC     .55
DEC     .6
DEC     .7
DEC     .8
```

```
DEC     .025
DEC     .03
DEC     .035
DEC     .04
DEC     .05
DEC     .06
DEC     .07
DEC     .08
DEC     .09
DEC     .1
DEC     .11
DEC     .12
DEC     .14
DEC     .16
DEC     .18
DEC     .2
DEC     .22
DEC     .24
DEC     .26
DEC     .28
DEC     .3
DEC     .32
DEC     .34
DEC     .36
DEC     .38
DEC     .4
```

```
DEC     .14
DEC     .16
DEC     .18
DEC     .2
DEC     .22
DEC     .24
DEC     .26
DEC     .28
DEC     .3
DEC     .32
DEC     .34
DEC     .36
DEC     .38
DEC     .4
DEC     .45
DEC     .5
DEC     .55
DEC     .6
DEC     .65
DEC     .7
DEC     .8
DEC     .9
DEC    1.
DEC    1.1
DEC    1.2
DEC    1.3
```

```
      DEC    .9
      DEC   1.
      DEC   1.1
      DEC   1.2
      DEC   1.3
      DEC   1.4
      DEC   1.6
      DEC   1.8
      DEC   2.
      DEC   2.2
      DEC   2.4
      DEC   2.6
      DEC   2.8
      DEC   3.
      DEC   3.2
      DEC   3.4
      DEC   3.6
      DEC   3.8
      DEC   4.
      DEC   4.5
      DEC   5.
      DEC   5.5
      DEC   6.
      DEC   6.5
      DEC   7.
POT   DEC   -29000.
```

```
      DEC    .45
      DEC    .5
      DEC    .55
      DEC    .6
      DEC    .7
      DEC    .8
      DEC    .9
      DEC   1.
      DEC   1.1
      DEC   1.2
      DEC   1.4
      DEC   1.6
      DEC   1.8
      DEC   2.
      DEC   2.2
      DEC   2.4
      DEC   2.6
      DEC   2.8
      DEC   3.
      DEC   3.2
      DEC   3.4
      DEC   3.6
      DEC   3.8
      DEC   4.
      DEC   4.5
      DEC   5.
```

```
      DEC   1.4
      DEC   1.5
      DEC   1.6
      DEC   1.8
      DEC   2.
      DEC   2.2
      DEC   2.4
      DEC   2.6
      DEC   2.8
      DEC   3.
      DEC   3.2
      DEC   3.4
      DEC   3.6
      DEC   3.8
      DEC   4.
      DEC   4.5
      DEC   5.
      DEC   5.5
      DEC   6
      DEC   6.5
      DEC   7.
POT   DEC   -79000.
      DEC   - 7004.
      DEC   - 3146.
      DEC   - 1907.
      DEC   - 1311.
```

```
      DEC   -11336.
      DEC   - 5539.4
      DEC   - 3610.
      DEC   - 2648.8
      DEC   - 2074.6
      DEC   - 1694.1
      DEC   - 1423.9
      DEC   - 1222.5
      DEC   -   943.2
      DEC   -   759.16
      DEC   -   629.14
      DEC   -   532.6
      DEC   -   458.28
      DEC   -   399.42
      DEC   -   312.54
      DEC   -   252.1
      DEC   -   208.14
      DEC   -   175.07
      DEC   -   149.49
      DEC   -   129.25
      DEC   -   112.9
      DEC   -    99.466
      DEC   -    88.248
      DEC   -    78.758
      DEC   -    60.448
      DEC   -    47.3
```

```
      DEC   5.5
      DEC   6.
      DEC   6.5
      DEC   7.
POT   DEC   -27820.
      DEC   -14880.
      DEC   - 9974.
      DEC     7410.
      DEC   - 5838.
      DEC   - 3890.
      DEC   - 2876.
      DEC   - 2258.
      DEC   - 1841.
      DEC   - 1543.
      DEC   - 1320.
      DEC   - 1019.
      DEC   -   818.4
      DEC   -   675.6
      DEC   -   569.4
      DEC   -   487.6
      DEC   -   423.2
      DEC   -   371.4
      DEC   -   329.
      DEC   -   265.6
      DEC   -   219.
      DEC   -   183.6
```

```
      DEC  -966.2
      DEC  -743.8
      DEC  -590.6
      DEC  -480.6
      DEC  -398.8
      DEC  -336.
      DEC  -286.6
      DEC  -246.8
      DEC  -214.2
      DEC  -187.1
      DEC  -164.3
      DEC  -144.9
      DEC  -128.4
      DEC  -114.3
      DEC  -102.2
      DEC  - 91.68
      DEC  - 71.3
      DEC  - 56.82
      DEC  - 46.24
      DEC  - 38.24
      DEC  - 32.06
      DEC  - 27.14
      DEC  - 19.88
      DEC  - 14.84
      DEC  - 11.25
      DEC  -  8.668
```

```
DEC   - 37.526
DEC   - 30.100
DEC   - 24.378
DEC   - 19.926
DEC   - 13.702
DEC   -  9.78
DEC   -  7.232
DEC   -  5.526
DEC   -  4.35
DEC   -  3.516
DEC   -  2.908
DEC   -  2.456
DEC   -  1.855
DEC   -  1.477
DEC   -  1.226
DEC   -  1.051
DEC   -   .9234
DEC   -   .8266
DEC   -   .7510
DEC   -   .6902
DEC   -   .6402
DEC   -   .598
DEC   -   .5616
DEC   -   .5302
DEC   -   .5024
DEC   -   .4452
```

```
DEC   - 156.
DEC   - 133.9
DEC   - 116.1
DEC   - 101.6
DEC   -  89.52
DEC   -  79.5
DEC   -  71.06
DEC   -  63.9
DEC   -  57.78
DEC   -  52.48
DEC   -  47.92
DEC   -  38.96
DEC   -  32.12
DEC   -  26.74
DEC   -  22.46
DEC   -  16.25
DEC   -  11.99
DEC   -   9.01
DEC   -   6.902
DEC   -   5.39
DEC   -   4.3
DEC   -   2.94
DEC   -   2.16
DEC   -   1.666
DEC   -   1.348
DEC   -   1.132
```

```
DEC   - 6.782
DEC   - 5.39
DEC   - 4.36
DEC   - 3.56
DEC   - 2.96
DEC   - 2.16
DEC   - 1.65
DEC   - 1.32
DEC   - 1.09
DEC   -  .936
DEC   -  .822
DEC   -  .736
DEC   -  .67
DEC   -  .618
DEC   -  .574
DEC   -  .538
DEC   -  .506
DEC   -  .446
DEC   -  .4
DEC   -  .364
DEC   -  .334
DEC   -  .308
DEC   -  .286
END
```

```
DEC    -   .4002
DEC    -   .3636
DEC    -   .3334
DEC    -   .3077
DEC    -   .2857
END
```

```
DEC    -   .98
DEC    -   .868
DEC    -   .782
DEC    -   .716
DEC    -   .662
DEC    -   .61
DEC    -   .57
DEC    -   .534
DEC    -   .504
DEC    -   .446
DEC    -   .4
DEC    -   .364
DEC    -   .334
DEC    -   .308
DEC    -   .286
END
```

Note 1: Note 1 to Appendix I also applies here

Note 2: Program prints ρ, R, $\frac{R}{\rho}$ and $\frac{dR}{d\rho}$ in decimal floating point along each line.

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